2,3,6-Trichlorophenylacetic acid sodium salt

2439-00-1 | DTXSID4041319

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.67e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.60e-01

Confidence level: 3.69e-01

Nearest Neighbors from the Training Set

Image not found
2,3-Dichlorobenzoic acid
Measured: 2.28e-04
Predicted: 2.49e-04

Image not found
p-Phenylazophenol
Measured: 4.72e-08
Predicted: 5.18e-07

Image not found
2,3,5-Trichlorobenzoic acid
Measured: 3.11e-04
Predicted: 1.83e-04

Image not found
alpha-Fenchone
Measured: 9.11e-04
Predicted: 5.32e-01

Image not found
2-Methylcyclohexanone
Measured: 9.95e-06
Predicted: 1.70